Summary of Working Group Session 2E: Materials Science*

- **Radiation damage of materials is inherently a multiscale phenomena and hence is well-suited for advanced simulations**
  - **Over 20 orders of magnitude time scale (10^{-14} to $>10^{6}$ s) and 10 orders of magnitude length scale (10^{-10} to 1 m)**
  - **Currently close to being able to perform simulations at the same length & time scale as experiments**
    - **There are clear near-term advances that can be achieved with leadership-class simulations**
- **Grand Challenge: Develop experimentally validated predictive performance models for materials in a hostile environment (high temperatures, damage levels/burnups, corrosive coolants)**
  - **Numerous corollary grand challenges were also discussed**
- **Long-term goal: reduce the fuel & material qualification time from current 10-15 year period to ~7 to 10 years, with reduced cost and increased confidence of extrapolation to untested regimes**
  - **Advanced simulations will be the key driver to achieving this goal, but experimental validation is also essential**

***Steve Zinkle, WG chair and Chuck Henager, rapporteur**

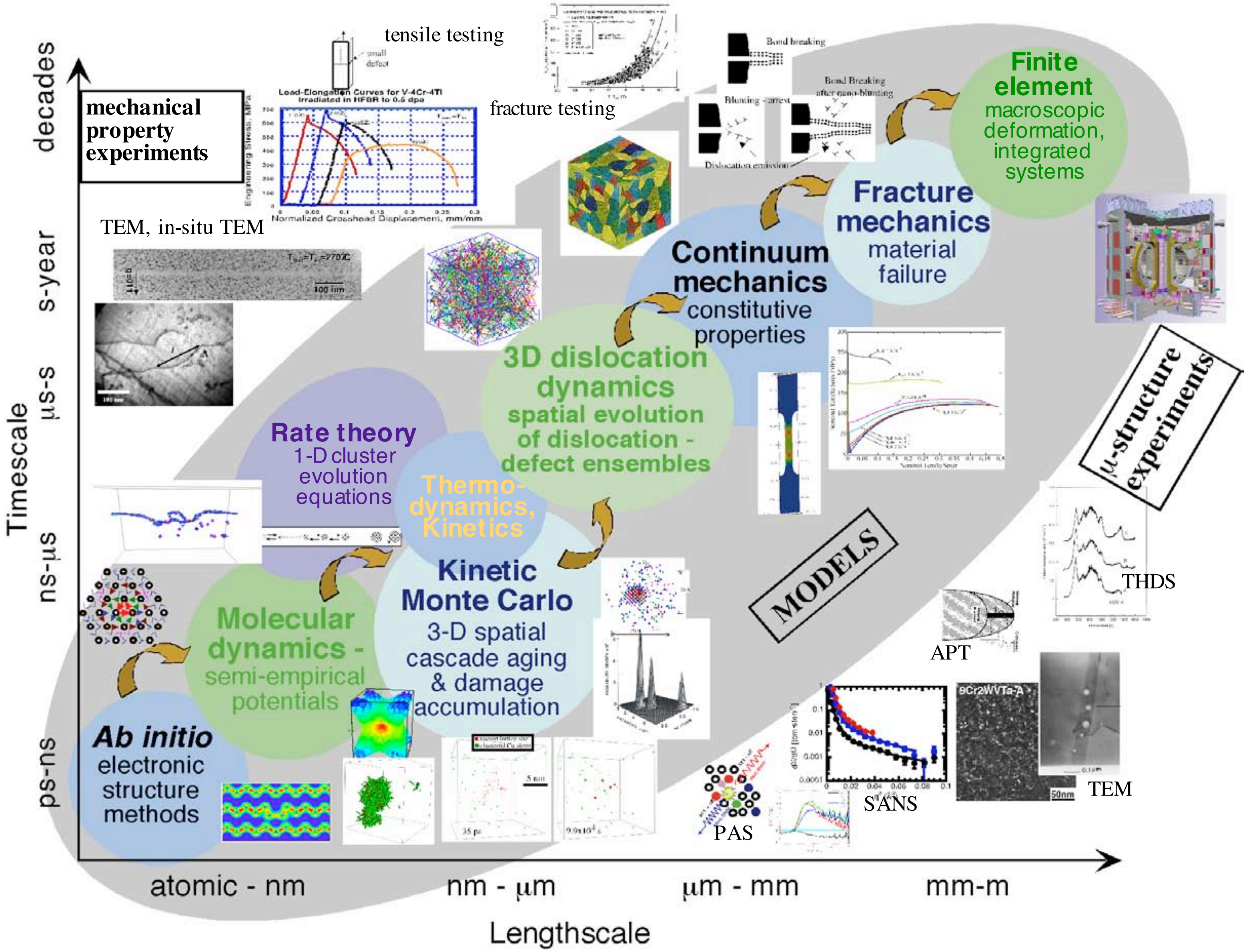
Summary of Working Group Session 2E: Materials Science *Cont'd*

- **Discussions covered structural materials (~65%), fuels (~25%), waste forms (~10%), and functional materials (<5%)**
- **Diversity of materials systems and broad range of time/length scales is both an asset and a hindrance**
  - **Numerous opportunities for commonality/complementarity leveraging with broader materials science modeling community**
  - **Practical logistic problems with investigation of too many materials and physical phenomena**
- **Extended discussion on multiscale code integration issues**
  - **Improved physics-based "coarse-graining" methodologies are needed to accurately pass information between length/time modeling scales**
    - **Existing codes are generally "stand-alone" platforms, not part of an integrated suite of codes**
  - **New paradigm?: Development of community-validated suite of standardized codes capable of running on various leadership-class computers**

Summary of Working Group Session 2E: Materials Science *Cont'd*

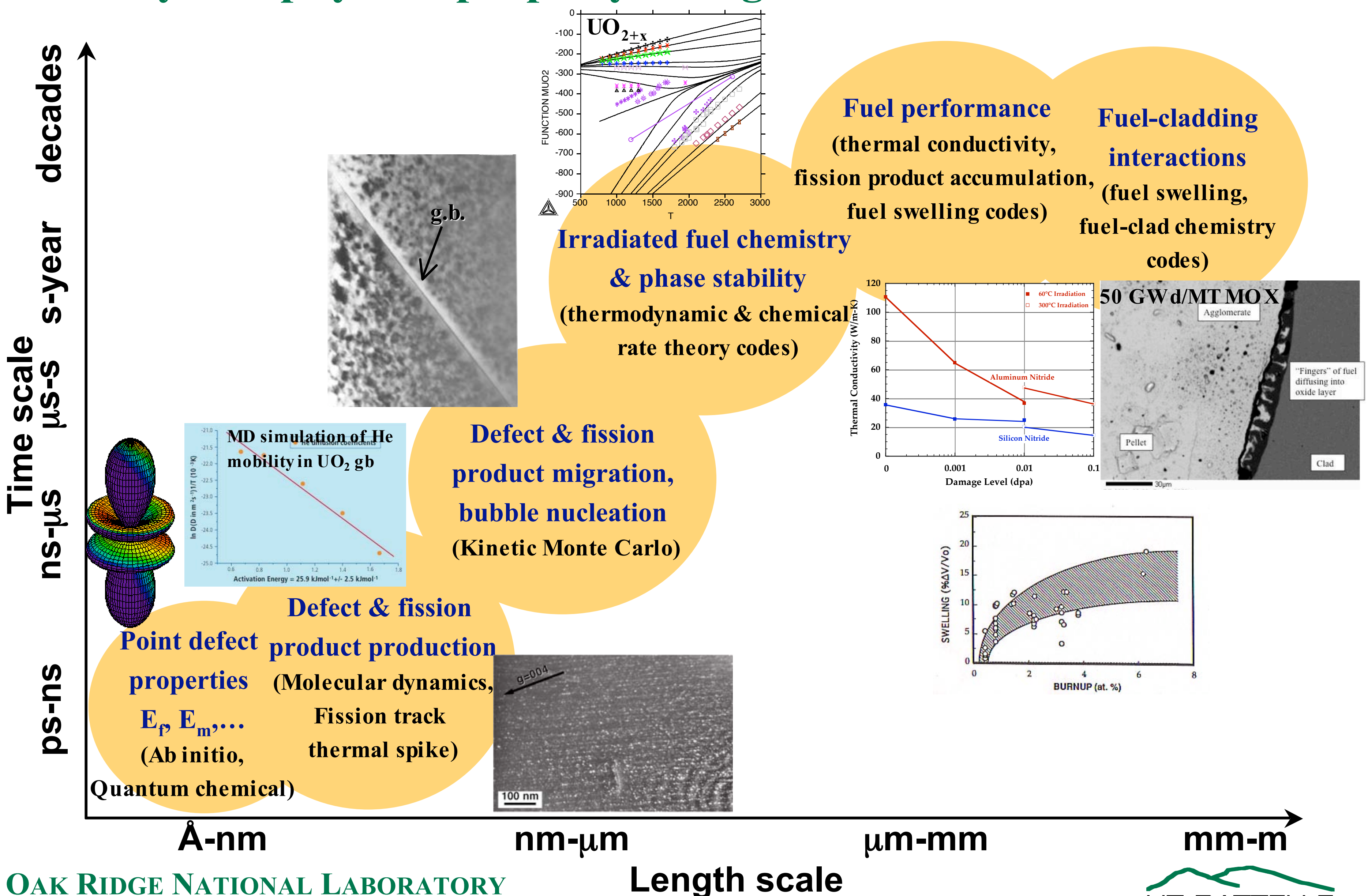
Material	Issues	Challenges	Near-term goals
Structural materials	Hardening/embrittlement Phase stability/RIS/IASCC Creep/swelling/fatigue He embrittlement	Microstructural evolution under radiation in order to predict properties	Fe-C interatomic potential Radiation-induced hardening via DD models Assess Gen. III alloys
Fuels	Modeling actinides Complex chemistry Fission products/damage Fuel performance code	Physics-based fuel performance code with thermodynamics and thermophysical props.	MOX phase stability including MA/fission products Model UO_2 microstructural evolution (incl. FP transport)
Waste Forms	Structure-property Impurities/stoichiometry Disorder Bonding	Phase stability under looooooong-term irradiation	Develop scientific basis for I, Tc sequestration (more tractable than current once-thru fuel cycle waste immobilization)
Functional materials	Electrical resistivity Optical properties Embrittlement	Suitable interatomic potentials Comput. framework for multiscale	

Radiation damage is inherently multiscale with interacting phenomena ranging from ps to decades and nm to m



B.D. Wirth, UC-Berkeley

Fission reactor fuels multiscale modeling places high emphasis on chemistry and physical property changes



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